



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 8, 2020 – 12:32 AM BST

PDB ID : 5L1B  
Title : AMPA subtype ionotropic glutamate receptor GluA2 in Apo state  
Authors : Yelshanskaya, M.V.; Singh, A.K.; Sampson, J.M.; Sobolevsky, A.I.  
Deposited on : 2016-07-28  
Resolution : 4.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at [validation@mail.wwpdb.org](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

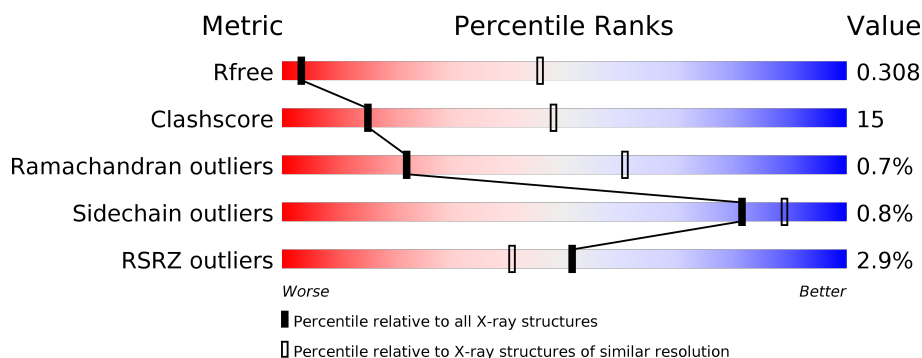
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

## *X-RAY DIFFRACTION*

The reported resolution of this entry is 4.00 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
$R_{free}$	130704	1087 (4.30-3.70)
Clashscore	141614	1148 (4.30-3.70)
Ramachandran outliers	138981	1108 (4.30-3.70)
Sidechain outliers	138945	1099 (4.30-3.70)
RSRZ outliers	127900	1028 (4.34-3.66)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	803	<div> <div>3%</div> <div> <div></div> <div>73%</div> <div>23%</div> <div>• •</div> </div> </div>
1	B	803	<div> <div>2%</div> <div> <div></div> <div>72%</div> <div>23%</div> <div>• •</div> </div> </div>
1	C	803	<div> <div>2%</div> <div> <div></div> <div>75%</div> <div>20%</div> <div>• •</div> </div> </div>
1	D	803	<div> <div>4%</div> <div> <div></div> <div>74%</div> <div>22%</div> <div>• •</div> </div> </div>

## 2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 24156 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Glutamate receptor 2, Glutamate receptor 2.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	780	Total	C	N	O	S	0	0	0
			6017	3865	995	1128	29			
1	B	780	Total	C	N	O	S	0	0	0
			6022	3868	995	1130	29			
1	C	780	Total	C	N	O	S	0	0	0
			6023	3868	995	1131	29			
1	D	783	Total	C	N	O	S	0	0	0
			6038	3875	998	1136	29			

There are 116 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	241	GLU	ASN	engineered mutation	UNP P19491
A	382	LEU	VAL	engineered mutation	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	THR	deletion	UNP P19491
A	?	-	GLU	deletion	UNP P19491
A	?	-	LEU	deletion	UNP P19491
A	?	-	PRO	deletion	UNP P19491
A	?	-	SER	deletion	UNP P19491
A	384	GLU	GLY	engineered mutation	UNP P19491
A	385	ASP	ASN	engineered mutation	UNP P19491
A	392	GLN	ASN	engineered mutation	UNP P19491
A	564	ASP	-	linker	UNP P19491
A	565	THR	-	linker	UNP P19491
A	566	ASP	-	linker	UNP P19491
A	589	ALA	CYS	engineered mutation	UNP P19491
A	744	THR	ASN	engineered mutation	UNP P19491
A	745	PRO	ALA	engineered mutation	UNP P19491
A	754	SER	ASN	engineered mutation	UNP P19491
A	758	VAL	LEU	engineered mutation	UNP P19491
A	775	ALA	SER	engineered mutation	UNP P19491
A	776	LYS	GLY	engineered mutation	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
A	777	ASP	GLY	engineered mutation	UNP P19491
A	778	SER	GLY	engineered mutation	UNP P19491
A	779	GLY	ASP	engineered mutation	UNP P19491
A	827	GLY	-	expression tag	UNP P19491
A	828	LEU	-	expression tag	UNP P19491
A	829	VAL	-	expression tag	UNP P19491
A	830	PRO	-	expression tag	UNP P19491
A	831	ARG	-	expression tag	UNP P19491
B	241	GLU	ASN	engineered mutation	UNP P19491
B	382	LEU	VAL	engineered mutation	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	THR	deletion	UNP P19491
B	?	-	GLU	deletion	UNP P19491
B	?	-	LEU	deletion	UNP P19491
B	?	-	PRO	deletion	UNP P19491
B	?	-	SER	deletion	UNP P19491
B	384	GLU	GLY	engineered mutation	UNP P19491
B	385	ASP	ASN	engineered mutation	UNP P19491
B	392	GLN	ASN	engineered mutation	UNP P19491
B	564	ASP	-	linker	UNP P19491
B	565	THR	-	linker	UNP P19491
B	566	ASP	-	linker	UNP P19491
B	589	ALA	CYS	engineered mutation	UNP P19491
B	744	THR	ASN	engineered mutation	UNP P19491
B	745	PRO	ALA	engineered mutation	UNP P19491
B	754	SER	ASN	engineered mutation	UNP P19491
B	758	VAL	LEU	engineered mutation	UNP P19491
B	775	ALA	SER	engineered mutation	UNP P19491
B	776	LYS	GLY	engineered mutation	UNP P19491
B	777	ASP	GLY	engineered mutation	UNP P19491
B	778	SER	GLY	engineered mutation	UNP P19491
B	779	GLY	ASP	engineered mutation	UNP P19491
B	827	GLY	-	expression tag	UNP P19491
B	828	LEU	-	expression tag	UNP P19491
B	829	VAL	-	expression tag	UNP P19491
B	830	PRO	-	expression tag	UNP P19491
B	831	ARG	-	expression tag	UNP P19491
C	241	GLU	ASN	engineered mutation	UNP P19491
C	382	LEU	VAL	engineered mutation	UNP P19491
C	?	-	LEU	deletion	UNP P19491
C	?	-	THR	deletion	UNP P19491
C	?	-	GLU	deletion	UNP P19491

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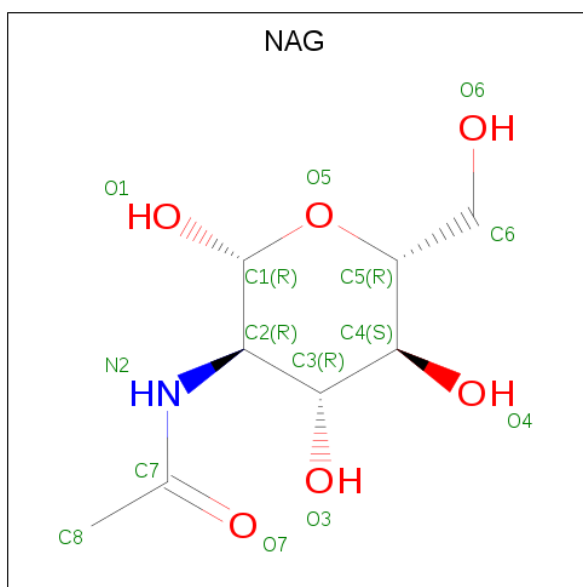
Chain	Residue	Modelled	Actual	Comment	Reference
C	?	-	LEU	deletion	UNP P19491
C	?	-	PRO	deletion	UNP P19491
C	?	-	SER	deletion	UNP P19491
C	384	GLU	GLY	engineered mutation	UNP P19491
C	385	ASP	ASN	engineered mutation	UNP P19491
C	392	GLN	ASN	engineered mutation	UNP P19491
C	564	ASP	-	linker	UNP P19491
C	565	THR	-	linker	UNP P19491
C	566	ASP	-	linker	UNP P19491
C	589	ALA	CYS	engineered mutation	UNP P19491
C	744	THR	ASN	engineered mutation	UNP P19491
C	745	PRO	ALA	engineered mutation	UNP P19491
C	754	SER	ASN	engineered mutation	UNP P19491
C	758	VAL	LEU	engineered mutation	UNP P19491
C	775	ALA	SER	engineered mutation	UNP P19491
C	776	LYS	GLY	engineered mutation	UNP P19491
C	777	ASP	GLY	engineered mutation	UNP P19491
C	778	SER	GLY	engineered mutation	UNP P19491
C	779	GLY	ASP	engineered mutation	UNP P19491
C	827	GLY	-	expression tag	UNP P19491
C	828	LEU	-	expression tag	UNP P19491
C	829	VAL	-	expression tag	UNP P19491
C	830	PRO	-	expression tag	UNP P19491
C	831	ARG	-	expression tag	UNP P19491
D	241	GLU	ASN	engineered mutation	UNP P19491
D	382	LEU	VAL	engineered mutation	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	THR	deletion	UNP P19491
D	?	-	GLU	deletion	UNP P19491
D	?	-	LEU	deletion	UNP P19491
D	?	-	PRO	deletion	UNP P19491
D	?	-	SER	deletion	UNP P19491
D	384	GLU	GLY	engineered mutation	UNP P19491
D	385	ASP	ASN	engineered mutation	UNP P19491
D	392	GLN	ASN	engineered mutation	UNP P19491
D	545	ASP	-	linker	UNP P19491
D	546	THR	-	linker	UNP P19491
D	547	ASP	-	linker	UNP P19491
D	589	ALA	CYS	engineered mutation	UNP P19491
D	744	THR	ASN	engineered mutation	UNP P19491
D	745	PRO	ALA	engineered mutation	UNP P19491
D	754	SER	ASN	engineered mutation	UNP P19491

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Chain	Residue	Modelled	Actual	Comment	Reference
D	758	VAL	LEU	engineered mutation	UNP P19491
D	775	ALA	SER	engineered mutation	UNP P19491
D	776	LYS	GLY	engineered mutation	UNP P19491
D	777	ASP	GLY	engineered mutation	UNP P19491
D	778	SER	GLY	engineered mutation	UNP P19491
D	779	GLY	ASP	engineered mutation	UNP P19491
D	827	GLY	-	expression tag	UNP P19491
D	828	LEU	-	expression tag	UNP P19491
D	829	VAL	-	expression tag	UNP P19491
D	830	PRO	-	expression tag	UNP P19491
D	831	ARG	-	expression tag	UNP P19491

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

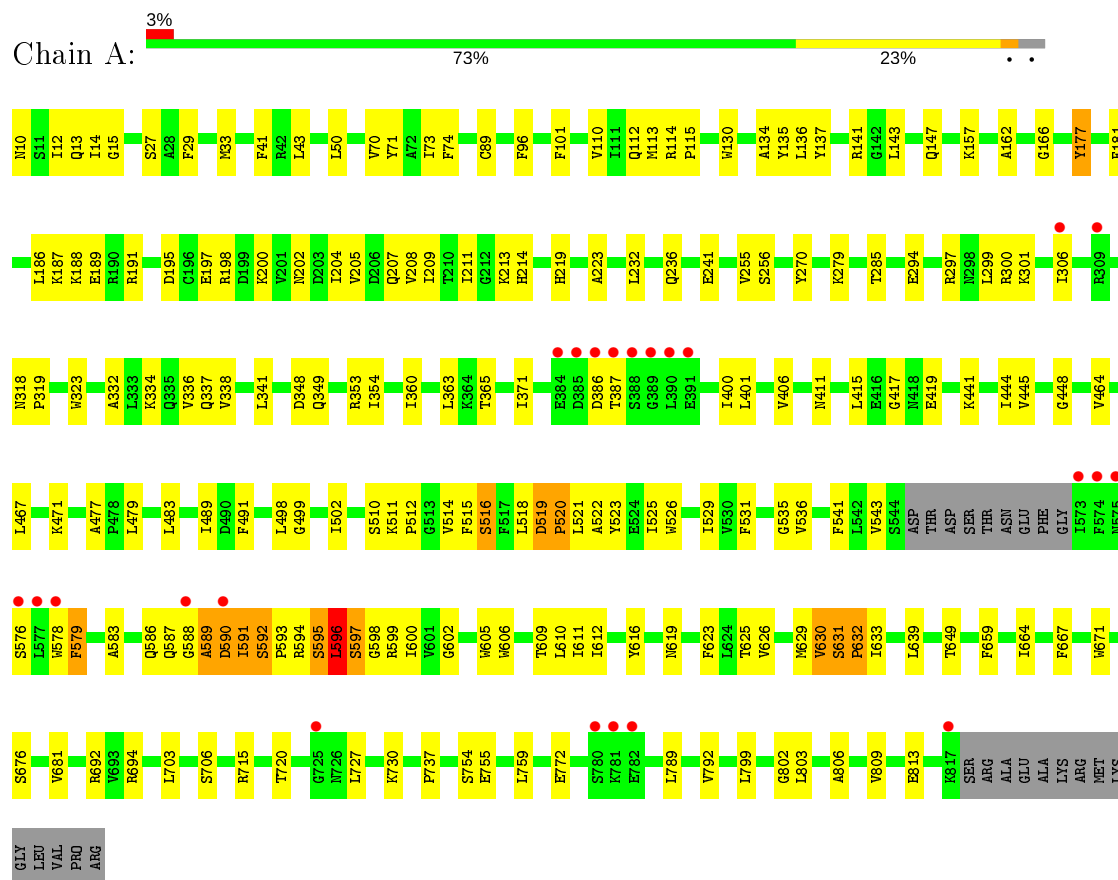


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			14	8	1	5		
2	B	1	Total	C	N	O	0	0
			14	8	1	5		
2	C	1	Total	C	N	O	0	0
			14	8	1	5		
2	D	1	Total	C	N	O	0	0
			14	8	1	5		

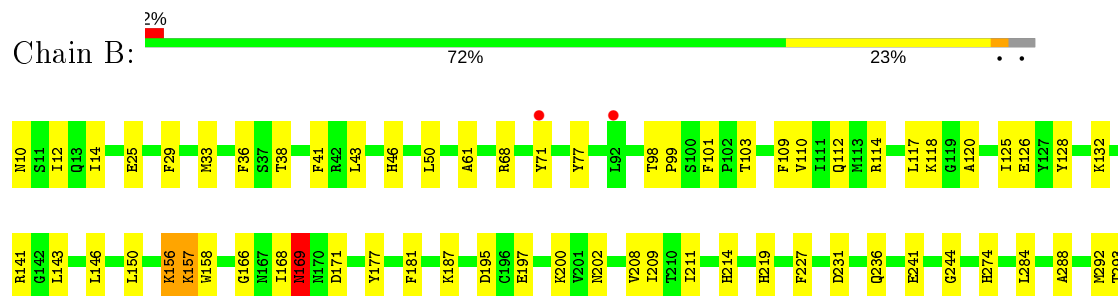
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density ( $RSRZ > 2$ ). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

- Molecule 1: Glutamate receptor 2, Glutamate receptor 2

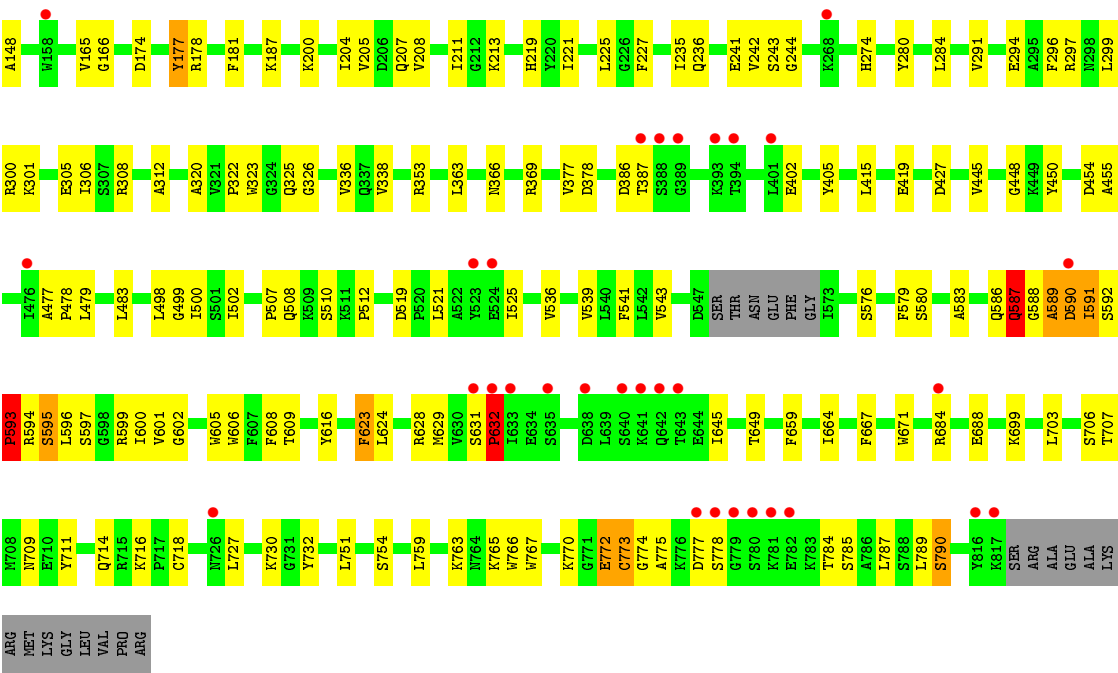


- Molecule 1: Glutamate receptor 2, Glutamate receptor 2









## 4 Data and refinement statistics

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	92.05Å 309.39Å 110.02Å 90.00° 93.77° 90.00°	Depositor
Resolution (Å)	48.55 – 4.00 48.55 – 4.00	Depositor EDS
% Data completeness (in resolution range)	97.7 (48.55-4.00) 97.7 (48.55-4.00)	Depositor EDS
$R_{merge}$	0.10	Depositor
$R_{sym}$	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	1.14 (at 4.00Å)	Xtriage
Refinement program	PHENIX 1.10.1 _2155	Depositor
R, $R_{free}$	0.265 , 0.292 0.286 , 0.308	Depositor DCC
$R_{free}$ test set	2522 reflections (5.00%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	175.2	Xtriage
Anisotropy	0.149	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.23 , 94.3	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.41$ , $\langle L^2 \rangle = 0.23$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
$F_o, F_c$ correlation	0.89	EDS
Total number of atoms	24156	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	180.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 3.19% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

## 5 Model quality

### 5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: NAG

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 5$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.35	2/6143 (0.0%)	0.62	14/8319 (0.2%)
1	B	0.35	3/6148 (0.0%)	0.74	22/8326 (0.3%)
1	C	0.50	4/6149 (0.1%)	0.69	26/8327 (0.3%)
1	D	0.41	4/6164 (0.1%)	0.62	14/8349 (0.2%)
All	All	0.41	13/24604 (0.1%)	0.67	76/33321 (0.2%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	B	0	1
1	D	0	3
All	All	0	4

All (13) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	520	PRO	N-CD	22.80	1.79	1.47
1	D	632	PRO	N-CD	22.49	1.79	1.47
1	A	632	PRO	N-CD	18.31	1.73	1.47
1	C	322	PRO	N-CD	-17.32	1.23	1.47
1	B	520	PRO	N-CD	15.40	1.69	1.47
1	C	632	PRO	N-CD	14.05	1.67	1.47
1	C	630	VAL	CA-C	8.21	1.74	1.52
1	B	632	PRO	N-CD	7.82	1.58	1.47
1	D	587	GLN	C-N	-7.10	1.20	1.33
1	D	631	SER	CA-C	5.74	1.67	1.52
1	B	623	PHE	CA-C	5.42	1.67	1.52
1	D	593	PRO	N-CD	5.37	1.55	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	520	PRO	N-CD	-5.01	1.40	1.47

All (76) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	589	ALA	CB-CA-C	-20.51	79.33	110.10
1	C	589	ALA	CB-CA-C	-20.01	80.09	110.10
1	A	589	ALA	CB-CA-C	-18.58	82.23	110.10
1	B	775	ALA	N-CA-C	18.00	159.61	111.00
1	B	775	ALA	CB-CA-C	-16.71	85.03	110.10
1	B	595	SER	CB-CA-C	-15.40	80.84	110.10
1	B	596	LEU	N-CA-CB	-15.18	80.03	110.40
1	C	589	ALA	N-CA-C	14.43	149.97	111.00
1	D	589	ALA	N-CA-C	14.17	149.26	111.00
1	A	589	ALA	N-CA-C	14.07	149.00	111.00
1	A	596	LEU	N-CA-CB	-13.19	84.02	110.40
1	B	776	LYS	N-CA-CB	-12.63	87.86	110.60
1	B	776	LYS	N-CA-C	12.39	144.45	111.00
1	A	595	SER	CB-CA-C	-12.03	87.25	110.10
1	D	790	SER	O-C-N	12.02	141.93	122.70
1	C	322	PRO	CA-N-CD	11.97	128.46	111.70
1	B	450	TYR	N-CA-C	11.94	143.25	111.00
1	C	595	SER	CB-CA-C	-11.71	87.84	110.10
1	B	589	ALA	CB-CA-C	-11.61	92.68	110.10
1	B	589	ALA	N-CA-C	11.41	141.82	111.00
1	C	520	PRO	CA-N-CD	-11.30	95.69	111.50
1	D	632	PRO	CA-N-CD	-11.24	95.76	111.50
1	B	595	SER	N-CA-C	11.14	141.08	111.00
1	C	596	LEU	N-CA-CB	-11.04	88.31	110.40
1	C	520	PRO	N-CA-CB	9.80	115.06	103.30
1	A	632	PRO	CA-N-CD	-9.75	97.85	111.50
1	D	590	ASP	N-CA-CB	-9.52	93.46	110.60
1	A	595	SER	N-CA-C	9.32	136.16	111.00
1	A	631	SER	C-N-CD	9.20	147.72	128.40
1	C	590	ASP	N-CA-CB	-9.11	94.20	110.60
1	D	790	SER	CA-C-N	-9.06	97.26	117.20
1	A	590	ASP	N-CA-CB	-8.97	94.46	110.60
1	B	450	TYR	CB-CA-C	-8.92	92.56	110.40
1	B	590	ASP	N-CA-CB	-8.69	94.96	110.60
1	D	587	GLN	O-C-N	-8.40	108.92	123.20
1	C	322	PRO	N-CA-CB	-8.34	93.29	103.30
1	B	520	PRO	CA-N-CD	-8.19	100.03	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	632	PRO	CA-N-CD	-8.17	100.06	111.50
1	B	624	LEU	N-CA-CB	7.82	126.04	110.40
1	D	61	ALA	N-CA-CB	7.82	121.05	110.10
1	A	597	SER	N-CA-CB	-7.81	98.78	110.50
1	C	631	SER	C-N-CD	7.71	144.58	128.40
1	B	623	PHE	CB-CA-C	-7.45	95.50	110.40
1	C	595	SER	N-CA-C	7.39	130.95	111.00
1	C	588	GLY	N-CA-C	7.36	131.50	113.10
1	C	510	SER	N-CA-C	7.21	130.46	111.00
1	B	156	LYS	N-CA-C	-7.03	92.02	111.00
1	C	630	VAL	CA-C-O	6.88	134.54	120.10
1	A	597	SER	N-CA-C	-6.79	92.66	111.00
1	D	632	PRO	N-CA-CB	6.76	111.41	103.30
1	C	630	VAL	CB-CA-C	-6.61	98.85	111.40
1	D	588	GLY	N-CA-C	6.51	129.37	113.10
1	A	630	VAL	CB-CA-C	-6.50	99.04	111.40
1	C	630	VAL	CA-C-N	-6.49	102.93	117.20
1	C	519	ASP	C-N-CD	6.45	141.93	128.40
1	A	632	PRO	N-CA-CB	6.34	110.91	103.30
1	C	519	ASP	CB-CA-C	-6.33	97.74	110.40
1	C	511	LYS	C-N-CD	6.10	141.20	128.40
1	D	587	GLN	CA-C-N	5.91	128.01	116.20
1	B	773	CYS	CB-CA-C	-5.89	98.63	110.40
1	A	630	VAL	N-CA-C	5.87	126.84	111.00
1	D	631	SER	CB-CA-C	5.70	120.94	110.10
1	B	596	LEU	N-CA-C	5.63	126.20	111.00
1	B	767	TRP	CB-CA-C	-5.40	99.60	110.40
1	C	519	ASP	CB-CG-OD2	5.32	123.08	118.30
1	D	590	ASP	N-CA-C	5.27	125.22	111.00
1	C	632	PRO	N-CA-CB	5.22	109.57	103.30
1	C	510	SER	CB-CA-C	-5.19	100.24	110.10
1	A	519	ASP	CB-CG-OD2	5.18	122.97	118.30
1	C	518	LEU	CB-CA-C	-5.17	100.38	110.20
1	B	519	ASP	CB-CG-OD2	5.16	122.94	118.30
1	C	590	ASP	N-CA-C	5.15	124.90	111.00
1	B	622	ALA	N-CA-C	5.13	124.86	111.00
1	B	623	PHE	CA-C-O	5.04	130.68	120.10
1	D	790	SER	C-N-CA	-5.02	109.16	121.70
1	C	518	LEU	N-CA-C	5.00	124.51	111.00

There are no chirality outliers.

All (4) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	B	450	TYR	Peptide
1	D	587	GLN	Mainchain
1	D	595	SER	Peptide
1	D	772	GLU	Peptide

## 5.2 Too-close contacts

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	6017	0	5899	210	1
1	B	6022	0	5906	212	1
1	C	6023	0	5907	180	0
1	D	6038	0	5906	218	0
2	A	14	0	13	1	0
2	B	14	0	13	0	0
2	C	14	0	13	0	0
2	D	14	0	13	0	0
All	All	24156	0	23670	718	1

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 15.

All (718) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:587:GLN:HE22	1:C:586:GLN:CB	1.01	1.55
1:D:711:TYR:HB2	1:D:767:TRP:CZ3	1.49	1.45
1:C:587:GLN:HE22	1:D:586:GLN:CB	1.29	1.43
1:A:632:PRO:N	1:A:632:PRO:CD	1.73	1.41
1:B:587:GLN:NE2	1:C:586:GLN:CB	1.74	1.41
1:B:520:PRO:CD	1:B:520:PRO:N	1.69	1.40
1:C:587:GLN:NE2	1:D:586:GLN:HB3	1.16	1.40
1:D:632:PRO:CD	1:D:632:PRO:N	1.79	1.39
1:C:632:PRO:CD	1:C:632:PRO:N	1.67	1.38
1:A:578:TRP:CB	1:D:596:LEU:CD1	2.02	1.36
1:A:578:TRP:CB	1:D:596:LEU:CD2	2.04	1.35
1:C:711:TYR:HB2	1:C:767:TRP:CZ3	1.60	1.35

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:520:PRO:CD	1:C:520:PRO:N	1.79	1.35
1:B:763:LYS:HE3	1:B:767:TRP:CZ3	1.60	1.33
1:B:126:GLU:OE2	1:B:156:LYS:NZ	1.65	1.29
1:C:587:GLN:NE2	1:D:586:GLN:CB	1.90	1.26
1:A:186:LEU:HB3	1:B:157:LYS:NZ	1.48	1.25
1:A:596:LEU:CD2	1:B:578:TRP:CB	2.15	1.24
1:B:587:GLN:NE2	1:C:586:GLN:HB2	1.31	1.23
1:D:594:ARG:O	1:D:596:LEU:HD12	1.08	1.20
1:C:626:VAL:HA	1:C:629:MET:HB2	1.23	1.17
1:A:623:PHE:CE1	1:B:785:SER:O	1.97	1.16
1:B:587:GLN:NE2	1:C:586:GLN:HB3	1.51	1.16
1:D:594:ARG:O	1:D:596:LEU:HA	1.44	1.15
1:A:619:ASN:ND2	1:A:623:PHE:HE2	1.40	1.14
1:B:763:LYS:HE3	1:B:767:TRP:CE3	1.84	1.11
1:D:716:LYS:N	1:D:772:GLU:OE1	1.82	1.11
1:A:578:TRP:CB	1:D:596:LEU:HD13	1.76	1.09
1:C:587:GLN:HE22	1:D:586:GLN:CA	1.65	1.08
1:A:578:TRP:CB	1:D:596:LEU:HD22	1.78	1.06
1:D:143:LEU:O	1:D:143:LEU:HD12	1.53	1.06
1:A:596:LEU:HD21	1:B:578:TRP:CB	1.86	1.06
1:A:186:LEU:CB	1:B:157:LYS:NZ	2.17	1.05
1:A:186:LEU:CB	1:B:157:LYS:HZ1	1.68	1.05
1:D:711:TYR:CB	1:D:767:TRP:HZ3	1.69	1.05
1:D:594:ARG:O	1:D:596:LEU:CD1	2.05	1.04
1:D:579:PHE:CZ	1:D:590:ASP:HB3	1.91	1.04
1:A:578:TRP:CB	1:D:596:LEU:HD21	1.87	1.04
1:A:587:GLN:HE22	1:B:586:GLN:HA	1.22	1.03
1:A:186:LEU:HB3	1:B:157:LYS:HZ1	0.86	1.02
1:A:578:TRP:CA	1:D:596:LEU:HD21	1.90	1.02
1:B:126:GLU:CD	1:B:156:LYS:NZ	2.13	1.01
1:A:633:ILE:HD12	1:A:633:ILE:H	1.17	1.01
1:A:578:TRP:CB	1:D:596:LEU:HD11	1.85	1.00
1:D:594:ARG:C	1:D:596:LEU:HD12	1.79	1.00
1:D:595:SER:HA	1:D:596:LEU:HD13	1.43	1.00
1:C:763:LYS:O	1:C:767:TRP:HD1	1.43	0.99
1:C:711:TYR:CB	1:C:767:TRP:HZ3	1.76	0.98
1:C:143:LEU:HD12	1:C:143:LEU:O	1.64	0.97
1:A:578:TRP:CA	1:D:596:LEU:HD11	1.94	0.97
1:A:595:SER:HA	1:A:596:LEU:HD22	1.47	0.97
1:B:143:LEU:HD23	1:B:146:LEU:HD23	1.44	0.96
1:D:579:PHE:HZ	1:D:590:ASP:HB3	1.23	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:619:ASN:ND2	1:A:623:PHE:CE2	2.33	0.95
1:A:578:TRP:HA	1:D:596:LEU:HD21	1.46	0.95
1:C:510:SER:C	1:C:512:PRO:HD3	1.86	0.95
1:C:630:VAL:O	1:C:630:VAL:HG12	1.67	0.95
1:C:623:PHE:HE1	1:D:785:SER:CB	1.80	0.95
1:A:578:TRP:CB	1:D:596:LEU:CG	2.45	0.94
1:D:711:TYR:CB	1:D:767:TRP:CZ3	2.45	0.93
1:A:619:ASN:HD21	1:A:623:PHE:HE2	1.05	0.93
1:C:198:ARG:HD3	1:C:279:LYS:HD2	1.49	0.92
1:A:596:LEU:HD23	1:B:578:TRP:CB	1.96	0.91
1:A:587:GLN:NE2	1:B:586:GLN:HA	1.85	0.91
1:A:623:PHE:HE1	1:B:785:SER:O	1.52	0.90
1:A:518:LEU:CD1	1:A:523:TYR:CZ	2.54	0.90
1:C:510:SER:O	1:C:512:PRO:HD3	1.72	0.89
1:B:157:LYS:O	1:B:158:TRP:CD1	2.25	0.89
1:B:763:LYS:CE	1:B:767:TRP:CE3	2.55	0.89
1:A:518:LEU:HD11	1:A:523:TYR:CZ	2.08	0.89
1:D:595:SER:HA	1:D:596:LEU:CD1	2.02	0.88
1:A:596:LEU:HD13	1:A:599:ARG:CB	2.05	0.86
1:A:498:LEU:HD11	1:A:730:LYS:CD	2.06	0.86
1:C:626:VAL:CA	1:C:629:MET:HB2	2.06	0.86
1:C:711:TYR:CB	1:C:767:TRP:CZ3	2.52	0.86
1:A:578:TRP:C	1:D:596:LEU:HD11	1.95	0.86
1:A:596:LEU:O	1:A:599:ARG:N	2.09	0.85
1:C:587:GLN:HE21	1:D:586:GLN:HB3	1.07	0.85
1:D:143:LEU:CD1	1:D:147:GLN:HG3	2.07	0.85
1:B:510:SER:N	1:B:629:MET:SD	2.52	0.83
1:B:763:LYS:CE	1:B:767:TRP:CZ3	2.55	0.83
1:C:763:LYS:O	1:C:767:TRP:CD1	2.31	0.83
1:B:518:LEU:HD12	1:B:519:ASP:N	1.94	0.82
1:A:596:LEU:HD21	1:B:578:TRP:C	2.01	0.81
1:B:143:LEU:CD2	1:B:146:LEU:HD23	2.10	0.81
1:A:518:LEU:CD1	1:A:523:TYR:CE1	2.64	0.81
1:A:596:LEU:CG	1:B:578:TRP:CB	2.58	0.81
1:C:143:LEU:HD21	1:D:143:LEU:HD21	1.60	0.81
1:A:578:TRP:O	1:D:596:LEU:HD11	1.81	0.80
1:C:711:TYR:HB2	1:C:767:TRP:HZ3	1.00	0.80
1:C:623:PHE:CE1	1:D:785:SER:HB3	2.16	0.80
1:B:714:GLN:HE22	1:B:775:ALA:HB3	1.45	0.80
1:D:143:LEU:CD1	1:D:143:LEU:O	2.30	0.80
1:D:592:SER:HB3	1:D:594:ARG:H	1.46	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:126:GLU:CD	1:B:156:LYS:HZ2	1.83	0.79
1:D:592:SER:HB3	1:D:594:ARG:N	1.98	0.79
1:C:587:GLN:HE22	1:D:586:GLN:HA	1.46	0.78
1:A:498:LEU:CD1	1:A:730:LYS:HG3	2.14	0.78
1:A:596:LEU:HG	1:B:578:TRP:CB	2.13	0.78
1:D:579:PHE:HZ	1:D:590:ASP:CB	1.98	0.77
1:C:623:PHE:CE1	1:D:785:SER:CB	2.65	0.77
1:A:510:SER:HB3	1:A:511:LYS:HA	1.66	0.77
1:A:518:LEU:HD13	1:A:523:TYR:CE1	2.19	0.77
1:C:630:VAL:O	1:C:631:SER:O	2.03	0.77
1:B:587:GLN:HE21	1:C:586:GLN:HB3	1.46	0.77
1:B:169:ASN:ND2	1:B:169:ASN:H	1.83	0.77
1:D:592:SER:N	1:D:593:PRO:HA	1.97	0.76
1:C:198:ARG:CD	1:C:279:LYS:HD2	2.14	0.76
1:A:518:LEU:HD13	1:A:523:TYR:CZ	2.21	0.76
1:B:132:LYS:NZ	1:B:187:LYS:HB3	2.02	0.75
1:C:649:THR:HG22	1:C:703:LEU:HB2	1.68	0.75
1:B:454:ASP:OD1	1:B:455:ALA:N	2.20	0.75
1:D:579:PHE:HZ	1:D:590:ASP:C	1.90	0.75
1:D:221:ILE:HG12	1:D:243:SER:HB2	1.66	0.74
1:C:166:GLY:HA2	1:C:200:LYS:NZ	2.03	0.73
1:A:602:GLY:HA2	1:A:605:TRP:HB3	1.70	0.73
1:C:498:LEU:HD12	1:C:499:GLY:N	2.02	0.73
1:D:763:LYS:O	1:D:767:TRP:HD1	1.72	0.73
1:A:623:PHE:CZ	1:B:785:SER:O	2.41	0.73
1:D:590:ASP:O	1:D:591:ILE:HG22	1.88	0.72
1:A:498:LEU:HD11	1:A:730:LYS:HD2	1.70	0.72
1:A:498:LEU:HD12	1:A:730:LYS:HG3	1.69	0.72
1:C:659:PHE:HB3	1:C:671:TRP:HB2	1.72	0.72
1:D:166:GLY:HA2	1:D:200:LYS:NZ	2.05	0.72
1:C:143:LEU:O	1:C:143:LEU:CD1	2.37	0.72
1:C:498:LEU:CD2	1:C:732:TYR:CE2	2.72	0.72
1:A:600:ILE:HG12	1:B:581:LEU:HD11	1.71	0.72
1:A:498:LEU:CD1	1:A:730:LYS:HD2	2.20	0.71
1:B:166:GLY:HA2	1:B:200:LYS:NZ	2.05	0.71
1:D:602:GLY:HA2	1:D:605:TRP:HB3	1.72	0.71
1:D:774:GLY:O	1:D:778:SER:N	2.20	0.71
1:C:510:SER:HA	1:C:511:LYS:CB	2.20	0.71
1:D:583:ALA:HB1	1:D:589:ALA:H	1.55	0.71
1:B:404:PRO:HG3	1:B:767:TRP:CD1	2.26	0.70
1:A:166:GLY:HA2	1:A:200:LYS:NZ	2.06	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:334:LYS:NZ	1:B:349:GLN:O	2.24	0.70
1:A:625:THR:O	1:A:629:MET:HG3	1.91	0.70
1:A:415:LEU:HD13	1:A:419:GLU:HB3	1.74	0.70
1:A:649:THR:HG22	1:A:703:LEU:HB2	1.72	0.70
1:C:579:PHE:HE2	1:C:590:ASP:HB3	1.56	0.70
1:C:498:LEU:CD1	1:C:730:LYS:HG3	2.21	0.69
1:C:143:LEU:CD2	1:D:143:LEU:HD21	2.21	0.69
1:A:755:GLU:OE2	1:D:483:LEU:N	2.26	0.69
1:D:579:PHE:CZ	1:D:590:ASP:C	2.66	0.69
1:B:404:PRO:CG	1:B:767:TRP:HE1	2.06	0.69
1:C:185:GLU:OE1	1:C:213:LYS:NZ	2.24	0.69
1:A:600:ILE:HG12	1:B:581:LEU:CD1	2.22	0.68
1:C:522:ALA:H	1:D:787:LEU:HD12	1.58	0.68
1:C:198:ARG:HE	1:C:229:ASP:HB3	1.58	0.68
1:B:157:LYS:O	1:B:158:TRP:HD1	1.75	0.68
1:C:619:ASN:OD1	1:D:624:LEU:HD13	1.93	0.68
1:C:213:LYS:O	1:C:220:TYR:OH	2.12	0.68
1:A:595:SER:HA	1:A:596:LEU:CD2	2.21	0.68
1:A:498:LEU:CD1	1:A:730:LYS:CD	2.72	0.67
1:B:103:THR:O	1:B:352:LYS:NZ	2.21	0.67
1:C:101:PHE:HA	1:C:114:ARG:HD2	1.75	0.67
1:B:498:LEU:HD21	1:B:732:TYR:CZ	2.29	0.67
1:B:766:TRP:O	1:B:767:TRP:HD1	1.77	0.67
1:D:366:ASN:HD21	1:D:369:ARG:HH11	1.43	0.67
1:D:60:ASN:OD1	1:D:61:ALA:N	2.28	0.67
1:B:38:THR:HG21	1:B:297:ARG:NH2	2.10	0.67
1:D:519:ASP:CG	1:D:623:PHE:HE2	1.98	0.67
1:D:628:ARG:N	1:D:629:MET:HA	2.10	0.67
1:A:519:ASP:HB2	1:A:520:PRO:HD3	1.76	0.66
1:C:626:VAL:HA	1:C:629:MET:CB	2.15	0.66
1:A:498:LEU:HD12	1:A:730:LYS:CG	2.25	0.66
1:C:587:GLN:NE2	1:D:586:GLN:HA	2.07	0.66
1:D:649:THR:HG22	1:D:703:LEU:HB2	1.77	0.66
1:D:166:GLY:HA2	1:D:200:LYS:HZ3	1.60	0.66
1:A:498:LEU:CD1	1:A:730:LYS:CG	2.74	0.66
1:B:498:LEU:CD1	1:B:730:LYS:HG3	2.25	0.65
1:C:623:PHE:HE1	1:D:785:SER:CA	2.08	0.65
1:A:596:LEU:CD1	1:A:599:ARG:CB	2.74	0.65
1:B:498:LEU:HD11	1:B:730:LYS:HD2	1.79	0.65
1:B:14:ILE:HD13	1:B:43:LEU:HD23	1.79	0.65
1:D:50:LEU:C	1:D:50:LEU:HD12	2.16	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:498:LEU:HD12	1:C:730:LYS:HG3	1.76	0.65
1:D:763:LYS:O	1:D:767:TRP:CD1	2.49	0.65
1:B:587:GLN:HE22	1:C:586:GLN:HB2	0.49	0.65
1:A:676:SER:OG	1:B:770:LYS:NZ	2.29	0.65
1:C:763:LYS:HD2	1:C:767:TRP:NE1	2.11	0.65
1:D:143:LEU:HD11	1:D:147:GLN:HE21	1.61	0.65
1:A:498:LEU:HD12	1:A:499:GLY:N	2.12	0.65
1:B:541:PHE:HD1	1:B:576:SER:HB3	1.62	0.65
1:C:498:LEU:HD11	1:C:730:LYS:CD	2.26	0.65
1:D:143:LEU:HD12	1:D:147:GLN:HG3	1.78	0.65
1:C:294:GLU:HG3	1:C:338:VAL:HG11	1.79	0.65
1:C:587:GLN:NE2	1:D:586:GLN:CA	2.40	0.65
1:A:596:LEU:HD21	1:B:578:TRP:CA	2.27	0.64
1:B:498:LEU:HD11	1:B:730:LYS:CD	2.27	0.64
1:C:510:SER:C	1:C:512:PRO:CD	2.65	0.64
1:D:498:LEU:HD22	1:D:707:THR:CG2	2.28	0.64
1:D:763:LYS:HD2	1:D:767:TRP:CD1	2.32	0.64
1:B:589:ALA:HB2	1:B:602:GLY:HA3	1.80	0.64
1:D:308:ARG:HE	1:D:312:ALA:HB2	1.63	0.64
1:C:763:LYS:HD2	1:C:767:TRP:CD1	2.32	0.63
1:C:590:ASP:O	1:C:591:ILE:HG22	1.98	0.63
1:D:143:LEU:HB2	1:D:146:LEU:HB3	1.79	0.63
1:B:38:THR:CG2	1:B:297:ARG:NH2	2.61	0.63
1:D:498:LEU:CD2	1:D:707:THR:CG2	2.75	0.63
1:A:518:LEU:HD11	1:A:523:TYR:OH	1.99	0.62
1:C:141:ARG:NH2	1:C:195:ASP:OD1	2.26	0.62
1:C:417:GLY:HA2	1:C:441:LYS:NZ	2.14	0.62
1:B:294:GLU:HG3	1:B:338:VAL:HG11	1.82	0.62
1:B:169:ASN:HD22	1:B:169:ASN:H	1.47	0.62
1:A:522:ALA:H	1:B:787:LEU:HD12	1.64	0.62
1:D:143:LEU:HD12	1:D:143:LEU:C	2.19	0.62
1:C:583:ALA:HB1	1:C:589:ALA:HA	1.82	0.62
1:B:586:GLN:HG3	1:B:586:GLN:O	2.00	0.61
1:C:166:GLY:HA2	1:C:200:LYS:HZ3	1.63	0.61
1:C:498:LEU:HD23	1:C:732:TYR:CE2	2.35	0.61
1:D:323:TRP:CZ3	1:D:326:GLY:N	2.68	0.61
1:A:181:PHE:HE2	1:A:208:VAL:HG22	1.64	0.61
1:A:595:SER:CA	1:A:596:LEU:HD22	2.28	0.61
1:A:518:LEU:HD11	1:A:523:TYR:CE1	2.34	0.61
1:D:594:ARG:C	1:D:596:LEU:CD1	2.64	0.61
1:A:166:GLY:HA2	1:A:200:LYS:HZ3	1.65	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:132:LYS:HZ1	1:B:187:LYS:HB3	1.65	0.60
1:B:404:PRO:HG3	1:B:767:TRP:NE1	2.16	0.60
1:A:596:LEU:HD21	1:B:578:TRP:O	2.00	0.60
1:D:219:HIS:CD2	1:D:241:GLU:HB2	2.36	0.60
1:A:294:GLU:HG3	1:A:338:VAL:HG11	1.81	0.60
1:B:642:GLN:HE22	1:B:645:ILE:HB	1.66	0.60
1:D:498:LEU:CD2	1:D:707:THR:HG23	2.31	0.60
1:B:498:LEU:HD12	1:B:730:LYS:CG	2.32	0.60
1:B:498:LEU:CD2	1:B:732:TYR:CZ	2.85	0.60
1:B:649:THR:HG22	1:B:703:LEU:HB2	1.83	0.60
1:D:519:ASP:OD1	1:D:623:PHE:HE2	1.84	0.60
1:B:166:GLY:HA2	1:B:200:LYS:HZ1	1.65	0.60
1:C:14:ILE:HD13	1:C:43:LEU:HD23	1.84	0.60
1:B:604:VAL:HG11	1:C:802:GLY:HA3	1.84	0.60
1:A:236:GLN:NE2	1:A:365:THR:O	2.32	0.60
1:A:143:LEU:HD12	1:A:143:LEU:O	2.02	0.60
1:B:50:LEU:C	1:B:50:LEU:HD12	2.22	0.60
1:A:543:VAL:HG11	1:A:597:SER:HB3	1.83	0.59
1:A:633:ILE:CD1	1:A:633:ILE:H	1.96	0.59
1:B:323:TRP:HZ3	1:B:325:GLN:HB2	1.66	0.59
1:D:498:LEU:HD22	1:D:707:THR:HG23	1.83	0.59
1:A:50:LEU:C	1:A:50:LEU:HD12	2.22	0.59
1:B:498:LEU:HD21	1:B:732:TYR:CE1	2.37	0.59
1:B:101:PHE:HA	1:B:114:ARG:HD2	1.84	0.59
1:B:99:PRO:HB3	1:B:284:LEU:HB2	1.84	0.59
1:C:579:PHE:CE2	1:C:590:ASP:HB3	2.37	0.59
1:C:722:LYS:NZ	1:C:724:GLY:O	2.35	0.59
1:D:323:TRP:HZ3	1:D:325:GLN:HB2	1.68	0.59
1:A:630:VAL:HG12	1:A:630:VAL:O	2.01	0.58
1:B:110:VAL:HG12	1:B:112:GLN:HG3	1.85	0.58
1:D:519:ASP:OD1	1:D:623:PHE:CE2	2.55	0.58
1:A:587:GLN:HE22	1:B:586:GLN:CA	2.05	0.58
1:C:143:LEU:HD12	1:C:143:LEU:C	2.23	0.58
1:B:236:GLN:NE2	1:B:365:THR:O	2.29	0.58
1:B:502:ILE:O	1:B:709:ASN:ND2	2.36	0.58
1:D:101:PHE:HA	1:D:114:ARG:HD2	1.86	0.58
1:B:274:HIS:ND1	1:B:274:HIS:O	2.35	0.58
1:D:765:LYS:O	1:D:770:LYS:HG2	2.04	0.58
1:D:402:GLU:OE1	1:D:450:TYR:OH	2.20	0.58
1:D:498:LEU:HD23	1:D:707:THR:HG21	1.86	0.57
1:A:141:ARG:NH2	1:A:195:ASP:OD1	2.23	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:803:LEU:HD21	1:D:536:VAL:HG22	1.86	0.57
1:A:510:SER:HB3	1:A:512:PRO:HD3	1.85	0.57
1:C:520:PRO:O	1:D:787:LEU:HG	2.05	0.57
1:B:498:LEU:HD12	1:B:730:LYS:HG3	1.84	0.57
1:D:308:ARG:NH2	1:D:323:TRP:NE1	2.52	0.57
1:A:143:LEU:HD22	1:B:143:LEU:HD22	1.85	0.57
1:D:118:LYS:HD2	1:D:148:ALA:HB2	1.87	0.57
1:B:202:ASN:HD21	1:B:231:ASP:H	1.52	0.57
1:B:498:LEU:CD1	1:B:730:LYS:CG	2.82	0.57
1:A:467:LEU:HD22	1:A:737:PRO:HD3	1.85	0.57
1:A:611:ILE:HG21	1:B:795:VAL:HG21	1.87	0.57
1:D:323:TRP:CZ3	1:D:325:GLN:HB2	2.39	0.57
1:A:543:VAL:CG1	1:A:597:SER:HB3	2.34	0.56
1:A:596:LEU:O	1:A:597:SER:C	2.42	0.56
1:C:498:LEU:HD12	1:C:730:LYS:CG	2.35	0.56
1:B:707:THR:HB	1:B:767:TRP:CH2	2.41	0.56
1:C:754:SER:HB2	1:C:759:LEU:HD12	1.87	0.56
1:D:579:PHE:CE2	1:D:591:ILE:HG22	2.41	0.56
1:A:464:VAL:HG13	1:A:489:ILE:HG12	1.87	0.56
1:B:412:HIS:CE1	1:B:413:GLU:HG3	2.40	0.56
1:D:132:LYS:HZ1	1:D:187:LYS:HB3	1.71	0.56
1:D:498:LEU:HD12	1:D:499:GLY:N	2.21	0.56
1:A:590:ASP:O	1:A:591:ILE:HG22	2.06	0.56
1:A:681:VAL:HA	1:A:692:ARG:HH12	1.71	0.56
1:A:186:LEU:HB2	1:B:157:LYS:NZ	2.15	0.56
1:B:606:TRP:HA	1:B:609:THR:HG22	1.87	0.56
1:C:274:HIS:ND1	1:C:274:HIS:O	2.39	0.56
1:A:587:GLN:OE1	1:B:586:GLN:HB3	2.05	0.56
1:B:529:ILE:HD12	1:B:612:ILE:HG21	1.87	0.56
1:B:587:GLN:CD	1:C:586:GLN:HB2	2.18	0.56
1:C:626:VAL:O	1:C:626:VAL:HG12	2.06	0.56
1:D:521:LEU:HD23	1:D:616:TYR:HD1	1.71	0.56
1:A:134:ALA:HB2	1:A:189:GLU:HG2	1.87	0.56
1:A:806:ALA:HA	1:D:600:ILE:HD11	1.86	0.56
1:D:454:ASP:OD1	1:D:455:ALA:N	2.39	0.56
1:C:143:LEU:HB2	1:C:146:LEU:HB3	1.88	0.56
1:A:633:ILE:HD12	1:A:633:ILE:N	2.02	0.56
1:A:754:SER:HB2	1:A:759:LEU:HD12	1.88	0.56
1:C:500:ILE:HB	1:C:727:LEU:HB2	1.87	0.56
1:D:628:ARG:H	1:D:629:MET:HA	1.70	0.56
1:A:583:ALA:HB1	1:A:589:ALA:H	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:626:VAL:O	1:A:630:VAL:HG23	2.06	0.55
1:C:170:ASN:HA	1:C:173:LYS:HB2	1.88	0.55
1:B:10:ASN:HB3	1:B:300:ARG:HH22	1.72	0.55
1:D:579:PHE:CZ	1:D:590:ASP:CB	2.76	0.55
1:D:102:PRO:HD3	1:D:114:ARG:HD2	1.87	0.55
1:A:14:ILE:HD13	1:A:43:LEU:HD23	1.88	0.55
1:A:15:GLY:HA3	1:A:73:ILE:HG12	1.87	0.55
1:A:659:PHE:HB3	1:A:671:TRP:HB2	1.87	0.55
1:B:500:ILE:HB	1:B:727:LEU:HB2	1.87	0.55
1:D:99:PRO:HB3	1:D:284:LEU:HB2	1.88	0.55
1:C:110:VAL:HG12	1:C:112:GLN:HG3	1.89	0.55
1:A:12:ILE:HG23	1:A:71:TYR:HD2	1.70	0.55
1:D:219:HIS:HA	1:D:241:GLU:O	2.06	0.55
1:D:579:PHE:CE2	1:D:590:ASP:O	2.60	0.55
1:B:480:THR:O	1:B:485:ARG:NH1	2.40	0.54
1:C:181:PHE:HE2	1:C:208:VAL:HG22	1.73	0.54
1:C:177:TYR:CD2	1:C:207:GLN:HG3	2.43	0.54
1:D:10:ASN:HB3	1:D:300:ARG:HH22	1.72	0.54
1:C:157:LYS:HD2	1:D:187:LYS:HE3	1.89	0.54
1:C:10:ASN:HB2	1:C:41:PHE:HA	1.89	0.54
1:B:498:LEU:CD1	1:B:730:LYS:HD2	2.38	0.54
1:C:174:ASP:O	1:C:178:ARG:NH1	2.41	0.54
1:D:583:ALA:HB1	1:D:589:ALA:N	2.22	0.54
1:C:510:SER:CA	1:C:511:LYS:CB	2.85	0.53
1:C:498:LEU:CD1	1:C:730:LYS:CG	2.86	0.53
1:D:177:TYR:CD2	1:D:207:GLN:HG3	2.42	0.53
1:D:580:SER:HA	1:D:583:ALA:HB3	1.89	0.53
1:D:594:ARG:HA	1:D:599:ARG:CB	2.38	0.53
1:B:504:ILE:HD12	1:B:632:PRO:HD2	1.89	0.53
1:C:642:GLN:HE22	1:C:645:ILE:HB	1.73	0.53
1:A:186:LEU:CB	1:B:157:LYS:HZ3	2.18	0.53
1:D:299:LEU:HD13	1:D:306:ILE:HG21	1.90	0.53
1:A:529:ILE:HD12	1:A:612:ILE:HG21	1.90	0.53
1:B:77:TYR:CE2	1:B:98:THR:HG21	2.43	0.53
1:C:103:THR:N	1:C:112:GLN:OE1	2.34	0.53
1:A:143:LEU:HD12	1:A:143:LEU:C	2.29	0.53
1:A:579:PHE:HE1	1:A:590:ASP:HB3	1.72	0.53
1:D:711:TYR:HB2	1:D:767:TRP:CE3	2.29	0.53
1:C:623:PHE:HE1	1:D:785:SER:HA	1.73	0.53
1:A:334:LYS:HZ3	1:A:349:GLN:C	2.12	0.53
1:B:323:TRP:CZ3	1:B:326:GLY:N	2.77	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:498:LEU:CD2	1:D:707:THR:HG21	2.38	0.53
1:A:595:SER:CA	1:A:596:LEU:CD2	2.86	0.53
1:D:659:PHE:HB3	1:D:671:TRP:HB2	1.90	0.53
1:B:404:PRO:CG	1:B:767:TRP:NE1	2.72	0.53
1:C:498:LEU:CD1	1:C:499:GLY:N	2.72	0.53
1:C:525:ILE:HG12	1:D:789:LEU:HD13	1.90	0.53
1:B:586:GLN:O	1:B:587:GLN:C	2.46	0.52
1:B:595:SER:HB2	1:C:575:ASN:HA	1.91	0.52
1:D:498:LEU:HD21	1:D:732:TYR:CZ	2.45	0.52
1:D:784:THR:HA	1:D:785:SER:HB2	1.90	0.52
1:C:498:LEU:CD1	1:C:730:LYS:CD	2.87	0.52
1:D:14:ILE:HD13	1:D:43:LEU:HD23	1.90	0.52
1:D:219:HIS:HD2	1:D:241:GLU:O	1.91	0.52
1:C:532:ALA:HB1	1:C:605:TRP:HZ3	1.73	0.52
1:B:36:PHE:HB3	1:B:293:THR:HG21	1.91	0.52
1:C:728:ASP:OD2	1:C:730:LYS:HE3	2.10	0.52
1:D:33:MET:HE1	1:D:43:LEU:HB2	1.92	0.52
1:A:181:PHE:CE2	1:A:208:VAL:HG22	2.44	0.52
1:D:770:LYS:N	1:D:770:LYS:CE	2.73	0.52
1:A:498:LEU:HD11	1:A:730:LYS:CG	2.40	0.52
1:B:522:ALA:HB3	1:B:525:ILE:HG13	1.92	0.52
1:B:775:ALA:HA	1:B:777:ASP:H	1.75	0.52
1:B:77:TYR:HE2	1:B:98:THR:HG21	1.75	0.52
1:B:50:LEU:CD2	1:B:61:ALA:CB	2.88	0.52
1:B:50:LEU:CD2	1:B:61:ALA:HB2	2.40	0.52
1:D:117:LEU:HD12	1:D:120:ALA:HB3	1.92	0.51
1:A:587:GLN:OE1	1:B:586:GLN:CB	2.58	0.51
1:A:610:LEU:HD21	1:B:613:ILE:HG21	1.91	0.51
1:D:132:LYS:NZ	1:D:187:LYS:HB3	2.25	0.51
1:D:77:TYR:CE2	1:D:98:THR:HG21	2.46	0.51
1:A:29:PHE:O	1:A:33:MET:HG2	2.11	0.51
1:B:639:LEU:HD23	1:B:639:LEU:O	2.10	0.51
1:B:707:THR:HA	1:B:767:TRP:CH2	2.46	0.51
1:B:775:ALA:N	1:B:777:ASP:H	2.08	0.51
1:D:629:MET:O	1:D:629:MET:HG2	2.11	0.51
1:A:188:LYS:NZ	1:A:471:LYS:NZ	2.59	0.51
1:B:132:LYS:HZ3	1:B:187:LYS:HB3	1.75	0.51
1:C:166:GLY:HA2	1:C:200:LYS:HZ1	1.75	0.51
1:D:498:LEU:HD12	1:D:730:LYS:HG3	1.92	0.51
1:D:592:SER:N	1:D:593:PRO:CA	2.72	0.51
1:A:401:LEU:HD23	1:A:406:VAL:HG12	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:809:VAL:HA	1:B:812:ILE:HG12	1.92	0.51
1:C:623:PHE:CE1	1:D:785:SER:HA	2.46	0.51
1:D:772:GLU:O	1:D:773:CYS:C	2.49	0.51
1:B:181:PHE:HD2	1:B:211:ILE:HD11	1.76	0.50
1:D:595:SER:CA	1:D:596:LEU:HD13	2.29	0.50
1:A:510:SER:HB3	1:A:511:LYS:CA	2.41	0.50
1:C:115:PRO:HA	1:C:353:ARG:HB2	1.93	0.50
1:B:707:THR:HB	1:B:767:TRP:HH2	1.76	0.50
1:D:498:LEU:HD23	1:D:707:THR:CG2	2.40	0.50
1:D:770:LYS:CA	1:D:770:LYS:HE2	2.41	0.50
1:C:291:VAL:HA	1:C:336:VAL:HG11	1.94	0.50
1:D:16:GLY:HA3	1:D:47:ILE:HD13	1.94	0.50
1:B:141:ARG:NH2	1:B:195:ASP:OD1	2.42	0.50
1:D:579:PHE:O	1:D:583:ALA:N	2.43	0.50
1:A:13:GLN:HG3	1:A:70:VAL:HG12	1.94	0.50
1:A:337:GLN:NE2	2:A:901:NAG:O7	2.37	0.50
1:B:635:SER:OG	1:B:638:ASP:OD1	2.30	0.50
1:A:630:VAL:O	1:A:630:VAL:CG1	2.57	0.50
1:C:498:LEU:CD1	1:C:730:LYS:HD2	2.42	0.50
1:B:359:ASN:HA	1:B:373:TYR:HA	1.92	0.50
1:C:221:ILE:HG12	1:C:243:SER:HB2	1.93	0.50
1:C:602:GLY:HA2	1:C:605:TRP:HB3	1.93	0.50
1:D:592:SER:OG	1:D:595:SER:C	2.50	0.50
1:B:763:LYS:HE2	1:B:767:TRP:CE3	2.43	0.49
1:C:77:TYR:CE2	1:C:98:THR:HG21	2.47	0.49
1:B:299:LEU:HD13	1:B:306:ILE:HG21	1.94	0.49
1:C:498:LEU:C	1:C:498:LEU:HD12	2.33	0.49
1:D:592:SER:CB	1:D:594:ARG:N	2.73	0.49
1:A:299:LEU:HD13	1:A:306:ILE:HG21	1.94	0.49
1:D:716:LYS:HG3	1:D:772:GLU:OE1	2.11	0.49
1:B:348:ASP:HB3	1:B:354:ILE:HD13	1.93	0.49
1:C:188:LYS:NZ	1:C:471:LYS:NZ	2.61	0.49
1:C:625:THR:O	1:C:629:MET:N	2.45	0.49
1:D:236:GLN:HG3	1:D:363:LEU:HD11	1.95	0.49
1:A:789:LEU:HD13	1:D:525:ILE:HG12	1.94	0.49
1:C:334:LYS:NZ	1:C:349:GLN:O	2.42	0.49
1:B:639:LEU:CD2	1:B:647:TYR:CD1	2.96	0.49
1:D:62:PHE:HE2	1:D:92:LEU:HD12	1.77	0.49
1:A:592:SER:HB2	1:A:598:GLY:HA3	1.93	0.49
1:B:602:GLY:HA2	1:B:605:TRP:HB3	1.95	0.49
1:C:169:ASN:ND2	1:C:172:LYS:HD3	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:518:LEU:CD2	1:A:523:TYR:CE1	2.95	0.49
1:B:117:LEU:HD12	1:B:120:ALA:HB3	1.95	0.49
1:A:600:ILE:CG1	1:B:581:LEU:CD1	2.90	0.49
1:D:118:LYS:HG2	1:D:145:THR:HA	1.94	0.49
1:B:417:GLY:HA2	1:B:441:LYS:NZ	2.28	0.49
1:B:597:SER:O	1:B:601:VAL:HG23	2.13	0.49
1:D:323:TRP:CZ3	1:D:325:GLN:C	2.86	0.49
1:B:405:TYR:CG	1:B:478:PRO:HG3	2.48	0.48
1:A:143:LEU:HD13	1:A:147:GLN:HG3	1.95	0.48
1:B:707:THR:CB	1:B:767:TRP:HH2	2.26	0.48
1:A:606:TRP:HA	1:A:609:THR:HG22	1.94	0.48
1:D:225:LEU:HB2	1:D:280:TYR:CD1	2.49	0.48
1:B:181:PHE:HE2	1:B:208:VAL:HG22	1.79	0.48
1:D:754:SER:HB2	1:D:759:LEU:HD12	1.95	0.48
1:C:231:ASP:HB3	1:C:234:LYS:HE2	1.95	0.48
1:D:305:GLU:O	1:D:325:GLN:HG2	2.14	0.48
1:D:594:ARG:C	1:D:596:LEU:HA	2.29	0.48
1:A:332:ALA:O	1:A:336:VAL:HG23	2.14	0.48
1:A:10:ASN:HB2	1:A:41:PHE:HA	1.96	0.48
1:C:402:GLU:OE1	1:C:450:TYR:OH	2.30	0.48
1:C:711:TYR:CA	1:C:767:TRP:HZ3	2.26	0.48
1:A:600:ILE:O	1:A:600:ILE:HG22	2.13	0.48
1:B:526:TRP:CE3	1:B:526:TRP:HA	2.48	0.48
1:D:512:PRO:HB3	1:D:790:SER:CB	2.44	0.48
1:A:113:MET:O	1:A:353:ARG:NH1	2.46	0.48
1:D:118:LYS:NZ	1:D:118:LYS:HB2	2.29	0.48
1:D:166:GLY:HA2	1:D:200:LYS:HZ1	1.79	0.48
1:D:386:ASP:HA	1:D:387:THR:HA	1.61	0.48
1:C:707:THR:HG21	1:C:732:TYR:HE2	1.79	0.47
1:D:714:GLN:HA	1:D:773:CYS:HB2	1.96	0.47
1:C:375:SER:HB3	1:C:378:ASP:HB2	1.95	0.47
1:A:181:PHE:HD2	1:A:211:ILE:HD11	1.78	0.47
1:A:792:VAL:HG21	1:D:525:ILE:HD13	1.96	0.47
1:C:242:VAL:HB	1:C:363:LEU:HB3	1.95	0.47
1:B:628:ARG:N	1:B:629:MET:HA	2.29	0.47
1:D:274:HIS:O	1:D:274:HIS:ND1	2.48	0.47
1:D:579:PHE:CZ	1:D:590:ASP:O	2.67	0.47
1:A:592:SER:OG	1:A:598:GLY:N	2.46	0.47
1:B:10:ASN:HB2	1:B:41:PHE:HA	1.96	0.47
1:C:62:PHE:HE2	1:C:92:LEU:HD12	1.80	0.47
1:D:415:LEU:HD13	1:D:419:GLU:HB3	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:664:ILE:HB	1:B:667:PHE:HD2	1.79	0.47
1:A:525:ILE:HG12	1:B:789:LEU:HD13	1.96	0.47
1:C:236:GLN:NE2	1:C:365:THR:O	2.46	0.47
1:A:255:VAL:HG13	1:A:341:LEU:HD22	1.97	0.47
1:A:541:PHE:HD2	1:A:576:SER:HB3	1.80	0.47
1:B:514:VAL:HG13	1:B:794:GLY:HA3	1.96	0.47
1:A:593:PRO:HB2	1:A:594:ARG:CB	2.45	0.47
1:B:498:LEU:HD12	1:B:498:LEU:C	2.35	0.47
1:B:498:LEU:HD12	1:B:499:GLY:N	2.30	0.47
1:D:294:GLU:HG3	1:D:338:VAL:HG11	1.97	0.47
1:D:477:ALA:O	1:D:479:LEU:N	2.47	0.47
1:A:499:GLY:O	1:A:706:SER:N	2.48	0.47
1:D:291:VAL:HA	1:D:336:VAL:HG11	1.97	0.47
1:D:592:SER:H	1:D:593:PRO:HA	1.78	0.47
1:B:126:GLU:CG	1:B:156:LYS:NZ	2.78	0.47
1:C:117:LEU:HD12	1:C:120:ALA:HB3	1.96	0.47
1:D:377:VAL:HG23	1:D:378:ASP:OD1	2.15	0.47
1:A:181:PHE:CD2	1:A:213:LYS:HD2	2.50	0.47
1:D:205:VAL:HG13	1:D:235:ILE:HG23	1.98	0.46
1:A:204:ILE:O	1:A:208:VAL:HG23	2.15	0.46
1:C:308:ARG:HE	1:C:312:ALA:HB2	1.80	0.46
1:C:715:ARG:HH11	1:C:772:GLU:HG3	1.80	0.46
1:B:775:ALA:HA	1:B:776:LYS:HA	1.45	0.46
1:C:425:CYS:HA	1:C:428:LEU:HB3	1.97	0.46
1:A:232:LEU:HB3	1:A:363:LEU:HD22	1.97	0.46
1:A:188:LYS:HZ1	1:A:471:LYS:NZ	2.14	0.46
1:A:525:ILE:HD13	1:B:792:VAL:HG21	1.98	0.46
1:C:498:LEU:HD21	1:C:732:TYR:CZ	2.51	0.46
1:D:235:ILE:HD12	1:D:242:VAL:HG21	1.97	0.46
1:D:308:ARG:NE	1:D:312:ALA:HB2	2.28	0.46
1:D:541:PHE:HD1	1:D:576:SER:HB3	1.80	0.46
1:A:521:LEU:HD22	1:A:526:TRP:CE2	2.51	0.46
1:C:715:ARG:NH1	1:C:772:GLU:HG3	2.31	0.46
1:D:165:VAL:HG21	1:D:204:ILE:HD11	1.98	0.46
1:D:579:PHE:HZ	1:D:590:ASP:CA	2.27	0.46
1:A:715:ARG:HH11	1:A:772:GLU:HG3	1.79	0.46
1:B:323:TRP:CZ3	1:B:325:GLN:HB2	2.49	0.46
1:C:103:THR:O	1:C:352:LYS:NZ	2.27	0.46
1:C:513:GLY:O	1:C:516:SER:OG	2.30	0.46
1:D:711:TYR:HB2	1:D:767:TRP:HZ3	0.81	0.46
1:D:62:PHE:CE2	1:D:88:PHE:HB3	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:583:ALA:HB1	1:A:589:ALA:N	2.30	0.46
1:B:528:CYS:HB3	1:C:796:PHE:CE2	2.51	0.46
1:C:290:GLN:HG2	1:C:338:VAL:HG21	1.98	0.46
1:A:348:ASP:HB3	1:A:354:ILE:HD13	1.97	0.45
1:B:209:ILE:HG23	1:B:214:HIS:NE2	2.32	0.45
1:B:386:ASP:HA	1:B:387:THR:HA	1.48	0.45
1:B:405:TYR:CD1	1:B:478:PRO:HG3	2.52	0.45
1:C:198:ARG:NE	1:C:229:ASP:HB3	2.29	0.45
1:D:135:TYR:CE2	1:D:137:TYR:HB3	2.52	0.45
1:D:181:PHE:HD2	1:D:213:LYS:HD2	1.82	0.45
1:D:115:PRO:HA	1:D:353:ARG:HB2	1.99	0.45
1:D:502:ILE:O	1:D:709:ASN:ND2	2.47	0.45
1:A:445:VAL:HG13	1:A:448:GLY:HA2	1.98	0.45
1:B:593:PRO:HB2	1:B:594:ARG:CB	2.46	0.45
1:D:498:LEU:CD1	1:D:730:LYS:HG3	2.47	0.45
1:A:619:ASN:O	1:A:623:PHE:HD2	1.99	0.45
1:C:118:LYS:HB2	1:C:118:LYS:NZ	2.32	0.45
1:D:297:ARG:HG2	1:D:301:LYS:HE3	1.99	0.45
1:D:427:ASP:OD2	1:D:766:TRP:NE1	2.46	0.45
1:D:770:LYS:N	1:D:770:LYS:HE2	2.31	0.45
1:A:130:TRP:CE2	1:A:191:ARG:HD3	2.52	0.45
1:B:766:TRP:O	1:B:767:TRP:CD1	2.65	0.45
1:C:102:PRO:HD3	1:C:114:ARG:HD2	1.97	0.45
1:A:74:PHE:CZ	1:A:285:THR:HG23	2.52	0.45
1:C:225:LEU:HB2	1:C:280:TYR:CD1	2.52	0.45
1:D:211:ILE:HG13	1:D:213:LYS:HG3	1.98	0.45
1:D:597:SER:O	1:D:601:VAL:HG23	2.17	0.45
1:A:360:ILE:O	1:A:371:ILE:HG22	2.16	0.45
1:A:521:LEU:HD12	1:A:616:TYR:HB2	1.98	0.45
1:A:101:PHE:HA	1:A:114:ARG:HD2	1.99	0.45
1:C:606:TRP:HA	1:C:609:THR:HG22	1.99	0.45
1:D:507:PRO:HA	1:D:508:GLN:HA	1.57	0.45
1:D:541:PHE:HA	1:D:576:SER:OG	2.16	0.45
1:B:498:LEU:CD1	1:B:730:LYS:CD	2.94	0.44
1:C:348:ASP:HB3	1:C:354:ILE:HD13	1.99	0.44
1:A:386:ASP:HA	1:A:387:THR:HA	1.74	0.44
1:B:586:GLN:C	1:B:587:GLN:HG2	2.37	0.44
1:C:131:ASP:OD1	1:C:131:ASP:N	2.50	0.44
1:C:412:HIS:CE1	1:C:413:GLU:HG3	2.52	0.44
1:A:483:LEU:HD13	1:D:751:LEU:HB2	1.99	0.44
1:A:50:LEU:HD12	1:A:50:LEU:O	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:586:GLN:HA	1:D:587:GLN:OE1	2.17	0.44
1:B:427:ASP:OD2	1:B:766:TRP:NE1	2.47	0.44
1:D:579:PHE:CE1	1:D:590:ASP:HB3	2.49	0.44
1:B:227:PHE:CD2	1:B:244:GLY:HA3	2.53	0.44
1:C:117:LEU:HD11	1:C:245:PHE:CD1	2.51	0.44
1:D:645:ILE:HG12	1:D:699:LYS:HA	1.99	0.44
1:A:198:ARG:HH21	1:A:279:LYS:HD3	1.82	0.44
1:A:400:ILE:HG22	1:A:477:ALA:HB1	1.99	0.44
1:B:297:ARG:HG2	1:B:301:LYS:HE3	1.99	0.44
1:C:321:VAL:HA	1:C:322:PRO:HD3	1.39	0.44
1:A:143:LEU:CD1	1:A:147:GLN:HG3	2.48	0.44
1:B:525:ILE:HD13	1:C:792:VAL:HG21	1.99	0.44
1:C:630:VAL:O	1:C:630:VAL:CG1	2.50	0.44
1:A:186:LEU:HD13	1:B:157:LYS:NZ	2.32	0.44
1:B:521:LEU:HA	1:C:787:LEU:HD23	1.99	0.44
1:D:320:ALA:O	1:D:322:PRO:HD3	2.18	0.44
1:A:515:PHE:CD1	1:A:518:LEU:HD21	2.52	0.44
1:A:518:LEU:HD12	1:A:518:LEU:O	2.18	0.44
1:B:481:ILE:HG12	1:B:491:PHE:CD1	2.53	0.44
1:B:474:ILE:HG13	1:B:736:THR:HG22	2.00	0.44
1:D:770:LYS:HA	1:D:770:LYS:HE2	1.99	0.44
1:C:174:ASP:OD1	1:C:207:GLN:NE2	2.42	0.44
1:D:500:ILE:HB	1:D:727:LEU:HB2	2.00	0.44
1:A:130:TRP:CD2	1:A:191:ARG:HD3	2.53	0.43
1:A:498:LEU:CD1	1:A:499:GLY:N	2.80	0.43
1:C:143:LEU:HD11	1:C:147:GLN:HE21	1.83	0.43
1:C:204:ILE:O	1:C:208:VAL:HG23	2.18	0.43
1:B:209:ILE:HG23	1:B:214:HIS:CE1	2.53	0.43
1:B:518:LEU:HB3	1:B:526:TRP:HE1	1.84	0.43
1:B:541:PHE:HA	1:B:576:SER:OG	2.18	0.43
1:C:188:LYS:NZ	1:C:471:LYS:HZ1	2.16	0.43
1:C:579:PHE:O	1:C:583:ALA:N	2.52	0.43
1:D:118:LYS:HZ1	1:D:118:LYS:HB2	1.83	0.43
1:D:60:ASN:OD1	1:D:60:ASN:C	2.55	0.43
1:D:774:GLY:O	1:D:777:ASP:N	2.51	0.43
1:A:297:ARG:HG2	1:A:301:LYS:HE3	2.01	0.43
1:B:25:GLU:N	1:B:25:GLU:OE1	2.49	0.43
1:C:297:ARG:HG2	1:C:301:LYS:HE3	2.00	0.43
1:C:684:ARG:N	1:C:688:GLU:OE1	2.44	0.43
1:D:227:PHE:CD2	1:D:244:GLY:HA3	2.53	0.43
1:D:579:PHE:CZ	1:D:591:ILE:HB	2.53	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:ILE:HD13	1:A:639:LEU:HD22	2.00	0.43
1:B:171:ASP:N	1:B:171:ASP:OD1	2.51	0.43
1:B:518:LEU:CB	1:B:526:TRP:HE1	2.31	0.43
1:D:181:PHE:CE2	1:D:208:VAL:HG22	2.54	0.43
1:B:518:LEU:HD12	1:B:519:ASP:CA	2.48	0.43
1:C:500:ILE:O	1:C:727:LEU:N	2.46	0.43
1:A:157:LYS:HD2	1:B:187:LYS:HE3	2.00	0.43
1:A:600:ILE:CG1	1:B:581:LEU:HD13	2.49	0.43
1:B:592:SER:N	1:B:593:PRO:HA	2.34	0.43
1:A:219:HIS:ND1	1:A:241:GLU:O	2.52	0.43
1:A:694:ARG:HE	1:A:720:THR:HG23	1.83	0.43
1:B:485:ARG:O	1:B:489:ILE:HG13	2.19	0.43
1:D:595:SER:CA	1:D:596:LEU:CD1	2.86	0.43
1:D:606:TRP:HA	1:D:609:THR:HG22	2.00	0.43
1:B:118:LYS:HB2	1:B:118:LYS:NZ	2.34	0.43
1:B:518:LEU:HD12	1:B:518:LEU:C	2.37	0.43
1:C:332:ALA:O	1:C:336:VAL:HG23	2.18	0.43
1:B:608:PHE:CG	1:C:799:LEU:HD22	2.54	0.43
1:C:169:ASN:HB2	1:C:171:ASP:OD1	2.18	0.42
1:A:667:PHE:HE1	1:A:727:LEU:HD13	1.84	0.42
1:B:219:HIS:HD2	1:B:241:GLU:O	2.02	0.42
1:C:171:ASP:N	1:C:171:ASP:OD1	2.46	0.42
1:A:479:LEU:HG	1:A:491:PHE:HZ	1.85	0.42
1:A:715:ARG:NH1	1:A:772:GLU:HG3	2.34	0.42
1:B:296:PHE:HD1	1:B:299:LEU:HD12	1.84	0.42
1:B:639:LEU:HD21	1:B:647:TYR:CD1	2.55	0.42
1:C:174:ASP:HA	1:C:207:GLN:HE22	1.84	0.42
1:B:575:ASN:OD1	1:B:576:SER:N	2.50	0.42
1:C:588:GLY:HA3	1:C:605:TRP:HD1	1.84	0.42
1:C:684:ARG:HB3	1:C:688:GLU:OE2	2.19	0.42
1:D:716:LYS:CB	1:D:772:GLU:OE1	2.67	0.42
1:B:50:LEU:O	1:B:50:LEU:HD12	2.19	0.42
1:C:585:MET:O	1:C:586:GLN:C	2.55	0.42
1:C:611:ILE:HA	1:C:611:ILE:HD13	1.92	0.42
1:D:13:GLN:HG3	1:D:70:VAL:HG12	2.00	0.42
1:A:578:TRP:HA	1:D:596:LEU:CD2	2.33	0.42
1:C:30:ARG:HB2	1:C:270:TYR:HE2	1.84	0.42
1:D:498:LEU:C	1:D:498:LEU:HD12	2.40	0.42
1:D:602:GLY:O	1:D:606:TRP:N	2.41	0.42
1:B:168:ILE:HD11	1:B:200:LYS:HE2	2.02	0.42
1:C:507:PRO:O	1:C:509:LYS:N	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:209:ILE:HA	1:A:214:HIS:CE1	2.55	0.41
1:B:624:LEU:HA	1:B:624:LEU:HD23	1.87	0.41
1:C:593:PRO:HB2	1:C:594:ARG:CB	2.50	0.41
1:D:499:GLY:O	1:D:706:SER:N	2.51	0.41
1:D:539:VAL:O	1:D:543:VAL:HG23	2.20	0.41
1:A:596:LEU:O	1:A:598:GLY:N	2.53	0.41
1:A:186:LEU:CD1	1:B:157:LYS:NZ	2.82	0.41
1:C:683:VAL:HB	1:C:688:GLU:HB2	2.01	0.41
1:D:323:TRP:HZ3	1:D:325:GLN:CB	2.31	0.41
1:A:181:PHE:CD2	1:A:211:ILE:HD11	2.54	0.41
1:A:195:ASP:HA	1:A:223:ALA:HB3	2.01	0.41
1:A:809:VAL:O	1:A:813:GLU:HG2	2.19	0.41
1:B:493:LYS:HD3	1:B:493:LYS:HA	1.90	0.41
1:C:498:LEU:HD21	1:C:732:TYR:CE2	2.55	0.41
1:D:10:ASN:HB2	1:D:41:PHE:HA	2.01	0.41
1:A:110:VAL:HG12	1:A:112:GLN:HG3	2.02	0.41
1:A:186:LEU:HB3	1:B:157:LYS:HZ2	1.67	0.41
1:A:115:PRO:HA	1:A:353:ARG:HB2	2.01	0.41
1:B:498:LEU:HD11	1:B:730:LYS:CG	2.49	0.41
1:B:518:LEU:O	1:B:521:LEU:HG	2.20	0.41
1:B:591:ILE:HD12	1:B:591:ILE:HA	1.95	0.41
1:D:22:ALA:HB1	1:D:25:GLU:HB2	2.01	0.41
1:A:202:ASN:HA	1:A:205:VAL:HB	2.02	0.41
1:A:417:GLY:HA2	1:A:441:LYS:NZ	2.35	0.41
1:A:593:PRO:HD2	1:A:595:SER:N	2.36	0.41
1:A:536:VAL:HG22	1:B:803:LEU:HD11	2.01	0.41
1:C:809:VAL:HA	1:C:812:ILE:HG12	2.01	0.41
1:D:445:VAL:HG13	1:D:448:GLY:HA2	2.03	0.41
1:B:125:ILE:H	1:B:125:ILE:HG13	1.72	0.41
1:C:196:CYS:HB3	1:C:200:LYS:HB3	2.03	0.41
1:B:611:ILE:HG21	1:C:795:VAL:HG21	2.02	0.41
1:D:174:ASP:O	1:D:178:ARG:HG3	2.21	0.41
1:D:405:TYR:CD1	1:D:478:PRO:HG3	2.56	0.41
1:A:177:TYR:CD2	1:A:207:GLN:HG3	2.56	0.41
1:B:12:ILE:HG23	1:B:71:TYR:HD1	1.85	0.41
1:B:109:PHE:HE2	1:B:327:VAL:HA	1.85	0.41
1:B:595:SER:HA	1:B:596:LEU:HA	1.96	0.41
1:B:754:SER:HB2	1:B:759:LEU:HD12	2.01	0.41
1:C:519:ASP:OD1	1:C:523:TYR:CE1	2.74	0.41
1:C:522:ALA:HB3	1:C:525:ILE:HG13	2.02	0.41
1:C:681:VAL:HA	1:C:692:ARG:HH12	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:684:ARG:HB3	1:D:688:GLU:OE2	2.21	0.41
1:A:587:GLN:HB2	1:A:588:GLY:H	1.64	0.41
1:A:89:CYS:SG	1:A:96:PHE:HB2	2.61	0.41
1:B:639:LEU:HD23	1:B:647:TYR:CD1	2.56	0.41
1:C:596:LEU:HG	1:C:596:LEU:O	2.21	0.41
1:A:799:LEU:HD22	1:D:608:PHE:CG	2.56	0.41
1:A:27:SER:HB3	1:A:270:TYR:HB3	2.02	0.41
1:A:589:ALA:HB3	1:B:585:MET:SD	2.61	0.41
1:B:29:PHE:O	1:B:33:MET:HG2	2.20	0.41
1:B:41:PHE:HZ	1:B:297:ARG:HB2	1.85	0.41
1:C:98:THR:HA	1:C:99:PRO:HD3	1.90	0.41
1:D:583:ALA:HB1	1:D:589:ALA:HA	2.02	0.41
1:C:524:GLU:HB3	1:D:789:LEU:HD22	2.03	0.41
1:A:135:TYR:CE2	1:A:137:TYR:HB3	2.56	0.41
1:A:514:VAL:O	1:A:515:PHE:C	2.57	0.41
1:B:46:HIS:NE2	1:B:68:ARG:NH1	2.68	0.41
1:C:483:LEU:O	1:C:487:GLU:HG3	2.21	0.41
1:A:802:GLY:O	1:A:806:ALA:N	2.46	0.41
1:B:401:LEU:HD23	1:B:406:VAL:HG12	2.02	0.41
1:B:483:LEU:HD13	1:C:751:LEU:HB2	2.02	0.41
1:C:664:ILE:HB	1:C:667:PHE:HD2	1.86	0.41
1:D:296:PHE:HD1	1:D:299:LEU:HD12	1.86	0.41
1:D:718:CYS:HB3	1:D:775:ALA:HB2	2.03	0.41
1:A:401:LEU:HG	1:A:444:ILE:HD12	2.03	0.40
1:A:600:ILE:CG2	1:A:600:ILE:O	2.69	0.40
1:B:288:ALA:O	1:B:292:MET:HG3	2.21	0.40
1:B:489:ILE:HD13	1:B:735:ALA:HB1	2.02	0.40
1:C:188:LYS:HZ1	1:C:471:LYS:NZ	2.19	0.40
1:A:10:ASN:HB3	1:A:300:ARG:HH22	1.85	0.40
1:A:411:ASN:OD1	1:A:411:ASN:N	2.55	0.40
1:A:162:ALA:HB3	1:B:150:LEU:HD22	2.04	0.40
1:C:498:LEU:HD11	1:C:730:LYS:HG3	2.00	0.40
1:C:522:ALA:N	1:D:787:LEU:HD12	2.31	0.40
1:A:516:SER:HA	1:A:519:ASP:OD2	2.22	0.40
1:A:531:PHE:O	1:A:535:GLY:N	2.52	0.40
1:A:592:SER:N	1:A:593:PRO:HA	2.37	0.40
1:A:600:ILE:HG12	1:B:581:LEU:CD2	2.51	0.40
1:B:128:TYR:CE1	1:B:219:HIS:HE1	2.40	0.40
1:B:399:THR:OG1	1:B:406:VAL:HG21	2.21	0.40
1:C:642:GLN:NE2	1:C:645:ILE:HB	2.35	0.40
1:D:664:ILE:HB	1:D:667:PHE:HD2	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:66:PHE:CZ	1:D:312:ALA:HB1	2.57	0.40
1:A:136:LEU:HD11	1:A:181:PHE:HE1	1.86	0.40
1:A:318:ASN:HA	1:A:319:PRO:HA	1.95	0.40
1:A:187:LYS:HE3	1:B:157:LYS:HG2	2.03	0.40
1:B:332:ALA:O	1:B:336:VAL:HG23	2.21	0.40
1:C:257:LYS:HE3	1:C:257:LYS:HB3	1.96	0.40
1:C:623:PHE:CE1	1:D:785:SER:CA	2.95	0.40
1:A:664:ILE:HB	1:A:667:PHE:HD2	1.87	0.40
1:B:479:LEU:HA	1:B:479:LEU:HD12	1.93	0.40

All (1) symmetry-related close contacts are listed below. The label for Atom-2 includes the symmetry operator and encoded unit-cell translations to be applied.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:SER:OG	1:B:469:TYR:OH[1_556]	2.19	0.01

## 5.3 Torsion angles [i](#)

### 5.3.1 Protein backbone [i](#)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	776/803 (97%)	721 (93%)	51 (7%)	4 (0%)	29	67
1	B	776/803 (97%)	716 (92%)	56 (7%)	4 (0%)	29	67
1	C	776/803 (97%)	722 (93%)	43 (6%)	11 (1%)	11	46
1	D	779/803 (97%)	724 (93%)	52 (7%)	3 (0%)	34	71
All	All	3107/3212 (97%)	2883 (93%)	202 (6%)	22 (1%)	22	61

All (22) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	516	SER

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Mol	Chain	Res	Type
1	C	511	LYS
1	C	585	MET
1	C	629	MET
1	C	631	SER
1	B	587	GLN
1	B	774	GLY
1	A	631	SER
1	B	169	ASN
1	C	508	GLN
1	D	591	ILE
1	D	22	ALA
1	D	510	SER
1	C	520	PRO
1	A	592	SER
1	C	512	PRO
1	C	592	SER
1	C	630	VAL
1	A	591	ILE
1	B	591	ILE
1	C	519	ASP
1	C	591	ILE

### 5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	631/683 (92%)	626 (99%)	5 (1%)	81	89
1	B	632/683 (92%)	626 (99%)	6 (1%)	78	88
1	C	633/683 (93%)	629 (99%)	4 (1%)	86	92
1	D	633/683 (93%)	628 (99%)	5 (1%)	81	89
All	All	2529/2732 (93%)	2509 (99%)	20 (1%)	81	89

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	177	TYR
1	A	197	GLU
1	A	323	TRP
1	A	579	PHE
1	A	596	LEU
1	B	157	LYS
1	B	169	ASN
1	B	177	TYR
1	B	197	GLU
1	B	517	PHE
1	B	526	TRP
1	C	177	TYR
1	C	323	TRP
1	C	510	SER
1	C	512	PRO
1	D	177	TYR
1	D	593	PRO
1	D	623	PHE
1	D	632	PRO
1	D	773	CYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	169	ASN
1	B	219	HIS
1	B	359	ASN
1	B	587	GLN
1	B	714	GLN
1	C	587	GLN
1	D	147	GLN
1	D	219	HIS

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

## 5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

## 5.5 Carbohydrates

There are no monosaccharides in this entry.

## 5.6 Ligand geometry

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z  > 2$	Counts	RMSZ	$\# Z  > 2$
2	NAG	C	901	1	14,14,15	0.21	0	17,19,21	0.44	0
2	NAG	B	901	1	14,14,15	0.25	0	17,19,21	0.40	0
2	NAG	D	901	1	14,14,15	0.21	0	17,19,21	0.43	0
2	NAG	A	901	1	14,14,15	0.18	0	17,19,21	0.45	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	C	901	1	-	2/6/23/26	0/1/1/1
2	NAG	B	901	1	-	0/6/23/26	0/1/1/1
2	NAG	D	901	1	-	1/6/23/26	0/1/1/1
2	NAG	A	901	1	-	0/6/23/26	0/1/1/1

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

All (3) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
2	C	901	NAG	C4-C5-C6-O6
2	C	901	NAG	O5-C5-C6-O6
2	D	901	NAG	O5-C5-C6-O6

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	901	NAG	1	0

## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
1	D	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	D	587:GLN	C	588:GLY	N	1.20

## 6 Fit of model and data

### 6.1 Protein, DNA and RNA chains

In the following table, the column labelled ‘#RSRZ> 2’ contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95<sup>th</sup> percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled ‘Q< 0.9’ lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å <sup>2</sup> )	Q<0.9
1	A	780/803 (97%)	-0.27	23 (2%)	51	41	93, 169, 256, 282	0
1	B	780/803 (97%)	-0.24	17 (2%)	62	52	92, 148, 268, 287	0
1	C	780/803 (97%)	-0.13	20 (2%)	56	46	93, 180, 264, 285	0
1	D	783/803 (97%)	-0.04	31 (3%)	38	30	94, 205, 257, 278	0
All	All	3123/3212 (97%)	-0.17	91 (2%)	51	41	92, 170, 260, 287	0

All (91) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	D	781	LYS	6.7
1	A	781	LYS	6.2
1	B	309	ARG	6.1
1	A	576	SER	5.4
1	D	779	GLY	4.6
1	D	777	ASP	4.5
1	A	573	ILE	4.4
1	A	389	GLY	4.3
1	A	575	ASN	4.1
1	D	780	SER	4.0
1	D	394	THR	3.9
1	D	817	LYS	3.9
1	D	778	SER	3.8
1	A	388	SER	3.8
1	B	306	ILE	3.7
1	C	309	ARG	3.7
1	D	476	ILE	3.7
1	D	640	SER	3.7
1	D	643	THR	3.6
1	C	306	ILE	3.6
1	C	325	GLN	3.5

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Mol	Chain	Res	Type	RSRZ
1	A	387	THR	3.5
1	C	780	SER	3.4
1	A	817	LYS	3.4
1	D	642	GLN	3.4
1	C	311	ASN	3.3
1	B	311	ASN	3.2
1	C	323	TRP	3.2
1	B	310	GLY	3.2
1	D	684	ARG	3.1
1	D	782	GLU	3.1
1	D	388	SER	3.1
1	C	544	SER	3.1
1	B	699	LYS	3.0
1	B	631	SER	3.0
1	A	309	ARG	2.9
1	A	574	PHE	2.9
1	A	384	GLU	2.9
1	B	630	VAL	2.9
1	C	72	ALA	2.8
1	D	401	LEU	2.8
1	A	780	SER	2.8
1	C	726	ASN	2.7
1	D	389	GLY	2.7
1	D	816	TYR	2.7
1	C	324	GLY	2.7
1	C	71	TYR	2.6
1	C	589	ALA	2.6
1	B	817	LYS	2.6
1	D	641	LYS	2.6
1	C	542	LEU	2.6
1	D	387	THR	2.6
1	A	578	TRP	2.6
1	A	386	ASP	2.5
1	D	632	PRO	2.5
1	A	391	GLU	2.5
1	B	698	GLY	2.5
1	D	635	SER	2.5
1	C	781	LYS	2.4
1	B	308	ARG	2.4
1	A	390	LEU	2.4
1	A	588	GLY	2.4
1	B	321	VAL	2.3

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Mol	Chain	Res	Type	RSRZ
1	B	71	TYR	2.3
1	A	782	GLU	2.3
1	A	577	LEU	2.3
1	A	385	ASP	2.3
1	A	590	ASP	2.3
1	C	328	GLU	2.3
1	A	306	ILE	2.2
1	B	780	SER	2.2
1	D	631	SER	2.2
1	B	644	GLU	2.2
1	C	308	ARG	2.2
1	D	523	TYR	2.2
1	D	158	TRP	2.2
1	D	524	GLU	2.1
1	B	816	TYR	2.1
1	D	590	ASP	2.1
1	D	268	LYS	2.1
1	D	633	ILE	2.1
1	B	781	LYS	2.1
1	C	541	PHE	2.1
1	D	638	ASP	2.1
1	C	811	LEU	2.1
1	A	725	GLY	2.1
1	B	92	LEU	2.1
1	C	592	SER	2.0
1	D	393	LYS	2.0
1	D	726	ASN	2.0
1	C	601	VAL	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains [i](#)

There are no non-standard protein/DNA/RNA residues in this entry.

## 6.3 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [i](#)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum,

median, 95<sup>th</sup> percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å <sup>2</sup> )	Q<0.9
2	NAG	A	901	14/15	0.87	0.24	217,217,217,217	0
2	NAG	C	901	14/15	0.89	0.19	259,259,259,259	0
2	NAG	D	901	14/15	0.90	0.22	216,216,216,216	0
2	NAG	B	901	14/15	0.91	0.19	239,239,239,239	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.